

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.48e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.77e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

Image not found

Pentachloroethane

Measured: 2.37e-03

Predicted: 2.48e-03

Image not found

1,2-Dibromo-3-chloropropane

Measured: 4.69e-03

Predicted: 2.20e-03

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1,2,2,3-Tetrachloropropane

Measured: 2.64e-03

Predicted: 5.54e-03

Image not found

Tetrachloroethylene

Measured: 1.21e-03

Predicted: 2.33e-03